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SCATTERING PROBLEMS IN NONRELATIVISTIC QUANTUM MECHANICS

PART I. ONE PARTICLE IN ONE DIMENSION

by

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ABSTRACT

Scattering problems are considered from the point of view of the mathematical questions involved, such as the boundary conditions and uniqueness of the solutions, and the determination of a Green's function. For simplicity, the treatment is confined to one-particle one-dimensional problems.

I. Introduction

A survey[1] of the voluminous literature on scattering suffices to show that one-particle scattering problems, or those which are effectively one-particle, e.g. two-particle scattering in the center-of-mass system, are apparently well formulated and the theory is in agreement with experiment. In many-particle problems, on the other hand, although some success has been achieved, the agreement between theory and experiment is often poor, particularly when exchange scattering is investigated. Moreover the mathematical procedures which have been devised to obtain numerical results in these many-body problems are not merely non-rigorous but appear often to contain internal inconsistencies.[2] The difficulties involved in deducing the experimentally very successful Breit-Wigner formula for nuclear reactions are well known[3]. Somewhat less well-known are the difficulties encountered when attempting to deduce a variational principle of the Schwinger type[4,5] for scattering with the inclusion of exchange. It has been conjectured[6] that in the problem of the scattering of electrons by hydrogen atoms, no iteration method stemming from the usual integral-equation formulation of the scattering problem can ever converge to give exchange scattering.

In our opinion the difficulties which have been mentioned stem in part from an incomplete understanding of the mathematical questions involved. It is these questions to which we devote our attention. Generally the solution of a scattering problem involves related difficulties concerning the boundary conditions, uniqueness, completeness, and the determination of a Green's function. There is a well-developed theory available for answering such questions about one-particle problems in one dimension. This theory can be extended to one-particle three-dimensional problems. The extension to many-particle problems is less immediate and, at this time, less rigorous. However, the one-particle problem furnishes a useful and clarifying guide toward the correct formulation in many-particle systems.

In this paper we shall consider one-particle one-dimensional systems. Many-dimensional many-particle cases will be treated in future reports.

The time-independent Schroedinger equation is

$$(1) \qquad \frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi \ ,$$

which we write in the form

$$(2) \qquad -\frac{d^2\psi}{dx^2} + q\psi = \lambda\psi ;$$

$$q = \frac{2mV}{\hbar^2} , \quad \lambda = \frac{2mE}{\hbar^2} .$$

In scattering problems we seek (for arbitrary positive λ) a solution of Eq. (2) which is continuous and possesses a continuous derivative over the entire interval $-\infty < x < \infty$. This solution is to have the form of an incident wave and a scattered part, as follows:

$$(3) \qquad \psi(x) = e^{i\sqrt{\lambda}\,x} + \phi(x) ,$$

where $\phi(x)$ is "everywhere outgoing at infinity", e.g.

$$(4) \qquad x \to \infty \ : \ \phi(x) \sim Ae^{i\sqrt{\lambda}x}$$

$$x \to -\infty \ : \ \phi(x) \sim Be^{-i\sqrt{\lambda}\,x} .$$

We shall show that the constants A and B are determined by the outgoing-wave condition. The transmission coefficient is $|A|^2$ and the reflection coefficient is $|B|^2$.

II. Boundary Conditions for a Finite Interval

Eq. (2) is the special case $p = 1$ of the equation

$$(5) \qquad \left[-\frac{d}{dx}\left(p\,\frac{d}{dx}\right) + q\right]\psi = \lambda\psi$$

which is itself a special case of

$$(6) \qquad (L - \lambda)\psi = 0,$$

where L is a linear operator. To make equation (6) meaningful it is necessary to specify the domain of L, i.e. the set of functions to which the operation L may be applied.

We shall assume that the operator L is considered in a finite interval (x_1,x_2), that $p(x)$ is continuous, differentiable and never zero in the closed interval (x_1,x_2), and that $q(x)$ is bounded in that interval. The domain of L will consist of those functions $v(x)$ which have piecewise continuous second derivatives in the interval (x_1,x_2) and for which the second derivatives are square integrable over (x_1,x_2).

We define a scalar produce of functions in the domain as follows:

$$[v,w] = \int_{x_1}^{x_2} v^* w\,dx . \tag{7}$$

Here the asterisk denotes complex conjugate. If we introduce the Wronskian $W(u_1,u_2)$ of two functions u_1,u_2 by the definition:

$$W(u_1,u_2) = u_1u_2' - u_2u_1' , \tag{8}$$

then integration by parts shows that

$$[v,Lw] - [Lv,w] = \left\{ pW(v^*,w) \right\} \Big|_{x_1}^{x_2} . \tag{9}$$

The symbol $\Big|_{x_1}^{x_2}$ indicates the difference between the values at $x = x_2$ and $x = x_1$ of the function to the left of the symbol.

Equation (9) is valid even if $q(x)$ has a jump discontinuity at a finite number of points. Such discontinuities occur, for example, in the quantum mechanical problem of scattering by a square well.

Now let us consider a subset D of the domain of L. D is such that the functions $v(x)$ in it satisfy the boundary conditions

$$v(x_1) + \alpha v'(x_1) = 0 , \tag{10}$$

$$v(x_2) + \beta v'(x_2) = 0 , \tag{11}$$

where α and β are arbitrary fixed real numbers, including possibly $\pm \infty$, and where the prime signifies the derivative. If v and w belong to the subset D, that is, if they both satisfy the boundary conditions (10) and (11), then from (9) we find that

$$[v,Lw] - [Lv,w] = 0 . \tag{12}$$

This expresses the fact that L is complex self-adjoint or hermitian.

The eigenfunctions $u(x)$ of the operator L are those functions in D which satisfy equation (5). In general, for arbitrary values of λ there will be no solution of (5) which satisfies both boundary conditions (10) and (11).

To find the eigenvalues and the eigenfunctions we start by constructing two solutions v_1 and v_2 of (5). $v_1(x_1,\lambda)$ satisfies the boundary condition (10), and $v_2(x_1,\lambda)$ satisfies the boundary condition (11). Then we shall investigate for what values of λ these two solutions are essentially the same.

Since equation (5) is a differential equation of the second order, a unique solution can be specified by giving the values of ψ and ψ' at $x = x_1$ or at $x = x_2$. To define a solution satisfying (10), it is sufficient to give $\psi'(x_1)$ an arbitrary value and then to put $\psi(x_1) = -\alpha\psi'(x_1)$. However, for later purposes it is important that the initial values of the solution be independent of the value of λ. This requirement can be satisfied in many ways. The following way is advantageous since it also makes sense if $\alpha = 0$ or $\alpha = \infty$: Put

$$v_1'(x_1,\lambda) = \frac{\alpha+1}{\alpha^2+1}, \quad v_1(x_1,\lambda) = -\frac{\alpha^2+\alpha}{\alpha^2+1}.$$

Besides $v_1(x,\lambda)$ the function $Cv_1(x,\lambda)$, where C is independent of x, is also a solution of (5) which satisfies (10). Conversely, any solution of (5) which satisfies (10) must be of the form $Cv_1(x,\lambda)$.

Similarly, we may define $v_2(x,\lambda)$ uniquely by putting

$$v_2'(x_2,\lambda) = \frac{\beta+1}{\beta^2+1}, \quad v_2(x_2,\lambda) = -\frac{\beta^2+\beta}{\beta^2+1}.$$

It is easily shown that both $v_1(x,\lambda)$ and $v_2(x,\lambda)$ are entire functions of λ for any fixed value of x.

In general, v_1 and v_2 are linearly independent functions. The eigenvalues of L are those values of λ for which v_1 and v_2 are linearly dependent, that is,

$$v_2 = Cv_1, \tag{13}$$

because if (13) is true then v_2 is a solution of (5) which satisfies (11) and also (10). Equation (13) is completely equivalent to the following:

$$W[v_1(x,\lambda),v_2(x,\lambda)] = 0 \tag{14}$$

Note that for a fixed value of λ, any two solutions ψ_1 and ψ_2 of (5) satisfy the relation

$$\frac{d}{dx}[pW(\psi_1,\psi_2)] = 0 \tag{15}$$

whether or not the boundary conditions (10) and (11) are satisfied; therefore, $pW[\psi_1(x,\lambda),\psi_2(x,\lambda)]$ is independent of x. Since p(x) is never zero in the interval, it is satisfied everywhere in the interval. Consequently, the zeroes of $W(v_1,v_2)$, as a function of λ, yield the eigenvalues of the operator

$$L = -\frac{d}{dx}\left(p\frac{d}{dx}\right) + q \tag{16}$$

considered on the set D. Note that because of (13) an eigenfunction $u_i(x,\lambda_i)$ corresponding to an eigenvalue λ_i is unique except for a multiplicative factor.

If u(x) is in D, then so is $u^*(x)$, since α and β in (10) and (11) are both real. In equation (12) put $v(x) = w(x) = u_i(x,\lambda_i)$; then we find that

$$(\lambda_i - \lambda_i^*)\,[u_i,u_i] = 0, \tag{17}$$

which implies that $\lambda_i - \lambda_i^* = 0$, that is, λ must be real. Similarly, if we put $v(x) = u_i(x,\lambda_i)w(x) = u_j(x,\lambda_j)$, where $\lambda_i \neq \lambda_j$, we obtain the orthogonality relation

$$[u_i,u_j] = 0. \tag{18}$$

III. Expansion Theorem for a Finite Interval

It can be proved[7] that the set of eigenfunctions u_i of L (Eq. (16)) is complete. More precisely, L has a denumerable set of eigenvalues λ_i with corresponding normalized quadratically integrable eigenfunctions u_i in the interval $x_1 \leq x \leq x_2$. Also, L is such that an arbitrary quadratically integrable function ψ can be expanded in terms of u_i as follows:

$$\psi = \sum_i a_i u_i. \tag{19}$$

Here

$$[u_i,u_j] = \delta_{ij} \tag{20}$$

and then

$$a_i = [u_i,\psi]. \tag{21}$$

It must be noted that Eq. (19) is true only in the sense that

$$\lim_{n\to\infty}\left[\psi - \sum_n a_n u_n,\ \psi - \sum a_n u_n\right] = 0. \tag{22}$$

For more restricted classes of functions the series (19) may converge everywhere, but not necessarily to the value of ψ, while for more restricted classes still, it may converge to the value of ψ at all points in the interval $x_1 \leq x \leq x_2$.

With the help of the following Schwarz inequality for any two quadratically integrable functions f,g:

$$[f,g]^2 \leq [f,f]\,[g,g], \tag{23}$$

we find that

$$\lim_{n\to\infty} \left[f, \sum_n a_n u_n \right] = [f,\psi] , \tag{24}$$

since

$$\lim_{n\to\infty} \left[f, \sum_n a_n u_n - \psi \right] \leq \lim_{n\to\infty} [f,f]^{\frac{1}{2}} \left[\psi - \sum_n a_n u_n,\ \psi - \sum_n a_n u_n \right]^{\frac{1}{2}} . \tag{25}$$

Thus for purposes of integration, the differences between ψ and $\sum_n a_n u_n$ may be ignored.

From (19) and (21) we conclude that we may write

$$\sum_i u_i(x)\, u_i^*(x') = \delta(x-x') \tag{26}$$

since for any ψ

$$\lim_{n\to\infty} \int dx' \sum_n u_n(x) u_n^*(x')\, \psi(x') = \lim_{n\to\infty} \sum_n a_n u_n(x) = \int_{x_1}^{x_2} dx \delta(x-x')\psi(x') . \tag{27}$$

It can also be demonstrated directly from the properties of the Green's function that

$$\lim_{n\to\infty} \sum \int dx \psi(x) u_n(x)\, u_n^*(x') = \psi(x') . \tag{28}$$

The Green's function $G(x,x',\lambda)$ is a solution of the equation

$$\left(-\frac{d}{dx} p \frac{d}{dx} + q - \lambda \right) G(x,x',\lambda) = \delta(x-x') \tag{29}$$

which satisfies the boundary conditions (7) and (8). Eq.(29) implies that $G(x,x',\lambda)$ has a discontimuity at $x = x'$ such that

$$\left[\frac{d}{dx} G(x,x',\lambda) \right] \Bigg|_{x'-0}^{x'+0} = -\frac{1}{p(x')} . \tag{30}$$

Remembering (11) we see that for $\lambda \neq \lambda_i$, $G(x,x',\lambda)$ can be written as

$$x < x' : G(x,x',\lambda) = - \frac{v_1(x,\lambda)v_2(x',\lambda)}{pW(v_1,v_2)}$$

(31)

$$x > x' : G(x,x',\lambda) = - \frac{v_2(x,\lambda)v_1(x',\lambda)}{pW(v_1,v_2)} \quad .$$

The functions v_1 and v_2 are defined as in section II.

For $\lambda = \lambda_i$, an eigenvalue of L, the zero of $pW(v_1,v_2)$ invalidates Eq. (31). This is to be expected since the homogeneous equation corresponding to Eq. (29) has a non-zero solution and therefore $\lambda = \lambda_i$. On the other hand if $\lambda \neq \lambda_i$, the Green's function exists and is unique. Its existence when $\lambda \neq \lambda_i$ is insured by the explicit construction of G in Eq. (31), and the uniqueness of this Green's function follows because if G_1 and G_2 are two solutions of Eq. (29) satisfying the boundary conditions, then $G = G_1 - G_2$ satisfies the boundary conditions and the equation

$$(32) \qquad \left(- \frac{d}{dx} p \frac{d}{dx} + q - \lambda \right) G(x,x',\lambda) = 0.$$

We have already shown that for $\lambda = \lambda_i$ there are no non-zero solutions to Eq. (32) (which is equivalent to Eq. (5)) satisfying the boundary conditions. Hence the Green's function is unique.

Combining Eq. (26) with Eq. (29) we obtain the following well-known expansion of the Green's function, valid for $\lambda = \lambda_i$:

$$(33) \qquad G(x,x',\lambda) = \sum_i \frac{u_i(x)\, u_i^*(x')}{\lambda_i - \lambda} \quad .$$

Eq. (31) shows that $G(x,x',\lambda) = G(x',x,\lambda)$. This symmetry is not manifested in Eq. (33), but it is implied, since in the problem we have been considering, $u_i(x)$ differs from a real function by a complex multiplicative factor only, and $u_i(x)u_i^*(x')$ is real. For the same reason the asterisk may be attached at will to either $u(x)$ or $u(x')$ in Equations (26) through (28).

We have thus far taken λ to be real. However, we can consider solutions of Eq. (5) for complex λ, and as we have already pointed out it can be shown that the functions $v_1(x,\lambda)$ and $v_2(x,\lambda)$ which satisfy the boundary condi-

tions (7) and (8) respectively and which are normalized independently are analytic functions of λ. Consequently $G(x,x',\lambda)$ as defined by Eqs. (29)-(31) is an analytic function of λ everywhere in the complex λ-plane except at eigenvalues $\lambda = \lambda_i$, where $G(x,x',\lambda)$ has a pole. The right side of Eq. (33) is similarly analytic, and hence we see by analytic continuation that Eq. (33) remains valid for complex λ. Moreover

$$(34) \qquad -\frac{1}{2\pi i}\int_C d\lambda G(x,x',\lambda) = \sum_i u_i(x)u_i^*(x') = \delta(x-x').$$

In Eq. (34), C is a positive (counter-clockwise) contour enclosing all the poles of $G(x,x',\lambda)$.

IV. Expansion Theorem for More General Operators

Equation (34) shows that the integration of the Green's function over a suitable contour in the complex λ-plane yields the complete set of normalized eigenfunctions of L. This result can be applied to more general types of operators, for example those having continuous spectra. Titchmarsh[8] has given a rigorous treatment of such operators using the theory of the Green's function. A summary of the theory, with applications to electromagnetic problems, has been given by Marcuvitz[9].

In what follows we shall discuss the method and give a few elementary examples by way of illustration. For a complete mathematical justification the reader is referred to Titchmarsh[8].

We start with the differential equation defining the Green's function, namely

$$(L - \lambda)G(x,x',\lambda) = \delta(x-x') ,$$

where L is some linear differential operator defined over some domain, and λ is an arbitrary complex number. The domain of L is to be chosen that L is complex self-adjoint.

Consider the integral of $G(x,x',\lambda)$ over a circle of radius R in the complex λ-plane. We put

$$(35) \qquad I_R = \frac{1}{2\pi i}\oint_R G(x,x',\lambda)\, d\lambda .$$

Eq. (34) shows that for the relatively simple operators considered so far, whose eigenfunctions form a complete set,

$$\lim_{R\to\infty} I_R = -\delta(x-x') \,. \tag{36}$$

For more general operators we must investigate the behavior of the Green's function for large values of λ and prove that (36) is correct. The Green's function continues to be constructed from those solutions of

$$(L - \lambda)\, u = 0 \tag{37}$$

which satisfy the boundary condition at one or the other end of the interval. By examining the behavior of these solutions for large λ, the validity of Eq. (36) can be established. For example, if we put $p = 1$ in Eq. (16) then the solutions $u(x,\lambda)$ generally behave like $e^{\pm i\sqrt{\lambda}\, x}$ for large $|\lambda|$, and we have the approximate relation

$$G(x,x') = -\frac{e^{i\sqrt{\lambda}\,|x-x'|}}{2i\sqrt{\lambda}} \,. \tag{38}$$

If we now put $\lambda = k^2$, we obtain

$$\lim I_R = \lim -\frac{1}{2\pi i}\oint \frac{e^{i\sqrt{\lambda}\,|x-x'|}}{2i\sqrt{\lambda}}\, d\lambda = -\frac{1}{2\pi}\int_{-\infty}^{\infty} dk e^{ik|x-x'|} = -\delta(x-x') \,.$$

Consequently, under these circumstances Eq. (36) has been established, and it is evidently quite generally true that Eq. (36) is valid if Eq. (38) holds for large $|\lambda|$.

Once (36) has been established, the circle of radius R can be modified into any suitable contour C. If $G(x,x',\lambda)$ has only poles, then C can be taken as a set of small circles, one around each pole, and thus by evaluating the residues we obtain the expansion of $\delta(x-x')$ as a sum of discrete eigenfunctions. If $G(x,x',\lambda)$ also has branch-point singularities, then C can be taken as the set of small circles around each pole plus contours around each of the branch cuts. From this contour we obtain the expansion of $\delta(x-x')$ as a sum of discrete eigenfunctions (residues from the poles) plus an integral of continuum eigenfunctions (the integrals over the cuts). These details will become clearer when the illustrations of the next section are considered.

From the expansion of the δ function, the expansion of any arbitrary function can be obtained as follows. Suppose that

$$\delta(x-x') = \sum u_i(x)\, u_i^*(x');$$

then, multiplying by $f(x')$ and integrating, we obtain

$$f(x) = \sum u_i(x) \int f(x')\, u_i^*(x')dx'.$$

V. Expansion Theorem. Illustrations for a Finite Interval

We present some examples in which the theory of the preceding section is used.

Choose $p = 1$, $q = 0$ in Eq. (5); then

$$L = -\frac{d^2}{dx^2} \quad . \tag{39}$$

Suppose that the interval is $0 \leq x \leq \pi$. The spectrum will of course depend on the boundary conditions. Thus if $v(0) = v(\pi) = 0$ are the boundary conditions, we have, for arbitrary complex λ

$$v_1(x,\lambda) = \sin \sqrt{\lambda}\, x \tag{40}$$

$$v_2(x,\lambda) = \sin \sqrt{\lambda}\, (x-\pi) \tag{41}$$

and, substituting in Eq. (31),

$$x < x' : G(x,x',\lambda) = -\frac{\sin x\sqrt{\lambda}\, \sin\, (x'-\pi)\sqrt{\lambda}}{\sqrt{\lambda}\, \sin\, \pi\sqrt{\lambda}}$$

$$x > x' : G(x,x',\lambda) = -\frac{\sin\, (x-\pi)\sqrt{\lambda}\, \sin\, x'\sqrt{\lambda}}{\sqrt{\lambda}\, \sin\, \pi\sqrt{\lambda}} \quad . \tag{42}$$

Note that for large values of $\lambda, 0 < \arg \lambda < 2\pi, G(x,x',\lambda)$ behaves like $e^{i\sqrt{\lambda}\,|x-x'|}/2i\sqrt{\lambda}$; consequently (36) can be proved valid. The poles of $G(x,x',\lambda)$ are at $\lambda = n^2$, n being any positive integer. There is no pole at $\lambda = 0$, where G is finite, nor is there a branch point at $\lambda = 0$, since although $\sqrt{\lambda}$ occurs in the numerator and denominator of G, $G(x,x',\lambda)$ returns to its original value as λ circles the origin. The contour C can be deformed to become the contour C' (Fig.1), so for arbitrary x,x', the evaluation of the integral (35) simply involves calculating the residues of G at the poles $\lambda' = n^2$.

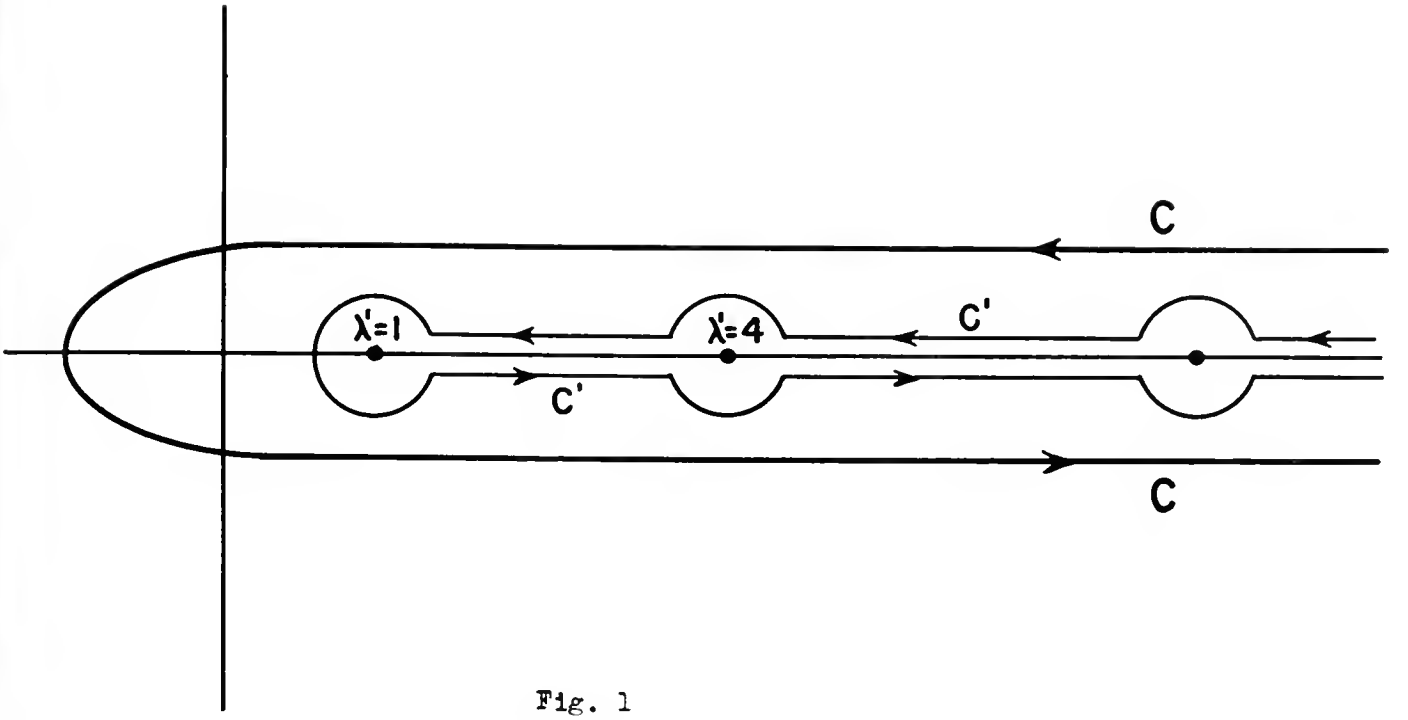

Fig. 1
Contour for $G(x,x',\lambda)$ of Eq. (42).

Using $G(x,x',\lambda)$ for $x < x'$, we obtain the following:

$$(43)\quad -\frac{1}{2\pi i}\int_C d\lambda G(x,x',\lambda) = \sum_n \frac{2}{\pi}\frac{\sin nx \sin n(x'-\pi)}{\cos n\pi} = \sum_{n=1}^{\infty}\frac{2}{\pi}\sin nx \sin nx'.$$

The normalized eigenfunctions are therefore

$$(44)\quad u_n(x) = \sqrt{\frac{2}{\pi}}\sin nx,$$

and in the interval $(0,\pi)$ an arbitrary square integrable function $f(x)$ has the expansion

$$(45)\quad f(x) = \frac{2}{\pi}\sum_{n=1}^{\infty}\sin nx\int_0^{\pi} dx'\, f(x')\sin nx'.$$

This is the well-known expansion in a series of sine functions.

If we choose the boundary conditions $v'(0) = v'(\pi) = 0$, then

$$(46)\quad \begin{aligned} v_1(x,\lambda) &= \cos\sqrt{\lambda}\, x \\ v_2(x,\lambda) &= \cos\sqrt{\lambda}\,(x-\pi) \\ W(v_1,v_2) &= \sqrt{\lambda}\sin\pi\sqrt{\lambda} \end{aligned}$$

$$x < x' : G(x,x',\lambda) = -\frac{\cos x\sqrt{\lambda}\cos(x'-\pi)\sqrt{\lambda}}{\sqrt{\lambda}\sin\pi\sqrt{\lambda}}$$

$$x > x' : G(x,x',\lambda) = -\frac{\cos(x-\pi)\sqrt{\lambda}\cos x'\sqrt{\lambda}}{\sqrt{\lambda}\sin\pi\sqrt{\lambda}}$$

The poles are at $\lambda = n^2$ and also at $\lambda = 0$. $G(x,x',\lambda)$ is single valued, and the contour is the same as in Fig. 1 above, except that the residue at $\lambda = 0$ must also be evaluated. Using Eq. (46) we have

$$(47) \qquad -\frac{1}{2\pi i}\int_C d\lambda\, G(x,x',\lambda) = \sum_{n=1}^{\infty} \frac{2}{\pi} \cos nx \cos nx' + \frac{1}{\pi}$$

which yields the following cosine expansion in the interval $(0,\pi)$:

$$(48) \qquad f(x) = \frac{1}{\pi}\int_0^{\pi} dx' f(x') + \frac{2}{\pi}\sum_{n=1}^{\infty} \cos nx \int_0^{\pi} dx' f(x') \cos nx'.$$

Eqs. (47) and (48) can of course be combined in the familiar way to obtain the expansion of an arbitrary function in the interval $(-\pi,\pi)$ in a series of sines and cosines. To obtain this expansion directly, it is necessary to impose periodic boundary conditions:

$$(49) \qquad \begin{aligned} u(-\pi) &= u(\pi) \\ u'(-\pi) &= u'(\pi). \end{aligned}$$

These so-called mixed boundary conditions are not of the form (7) and (8). However, it is easy to see from Eq. (10) that Eq. (49) still guarantees Eq. (12). Consequently the operator $L = -\frac{d^2}{dx^2}$ remains hermitian self-adjoint.

We can find the expansion theorem for L in the domain defined by (49) by the method of the preceding section. Since independent solutions of the differential equation

$$u'' + \lambda u = 0$$

are $\sin\sqrt{\lambda}\, x$ and $\cos\sqrt{\lambda}\, x$, we may assume that

$$(50) \qquad \begin{aligned} G(x,x',\lambda) &= a \sin\sqrt{\lambda}\, x + b \cos\sqrt{\lambda}\, y, \quad x < x' \\ &= c \sin\sqrt{\lambda}\, x + d \cos\sqrt{\lambda}\, y, \quad x > x'. \end{aligned}$$

The coefficients a, b, c, d, are determined by the boundary conditions (49) and by equation (30). We find that

$$(51) \qquad \begin{aligned} G(x,x',\lambda) &= -\frac{\cos\sqrt{\lambda}\, x \cos\sqrt{\lambda}(\pi - x') - \sin\sqrt{\lambda}\, x \sin\sqrt{\lambda}(\pi - x')}{2\sqrt{\lambda}\sin\pi\sqrt{\lambda}}, \quad x < x' \\ &= -\frac{\cos\sqrt{\lambda}\, x \cos\sqrt{\lambda}(\pi + x') + \sin\sqrt{\lambda}\, x \sin\sqrt{\lambda}(\pi + x')}{2\sqrt{\lambda}\sin\pi\sqrt{\lambda}}, \quad x > x'. \end{aligned}$$

The contour and the singularities of the Green's function are the same as in the

case of the cosine series above. We obtain

$$-\frac{1}{2\pi i}\int d\lambda G(x,x',\lambda) = \frac{1}{\pi}\sum_{n=1}^{\infty}(\cos nx \cos nx' + \sin nx \sin nx') + \frac{1}{2\pi} ,$$

and this implies that

$$f(x) = \frac{1}{2\pi}\int_{-\pi}^{\pi} dx' f(x') + \frac{1}{\pi}\sum_{1}^{\infty}\left\{\cos nx \int_{-\pi}^{\pi} dx' f(x')\cos nx' + \sin nx \int_{-\pi}^{\pi} dx' f(x')\sin nx'\right\} .$$

This example is very helpful in illustrating what occurs with the Green's function in more than one dimension. We see that $G(x,x',\lambda)$ may not be of the simple form given by (31), namely a function of x multiplied by a function of x' and divided by a function of λ. Instead, as is shown in Eq. (51), the Green's function may be a sum of products of functions of x and functions of x', all divided by a function of λ. In such a case each term in the sum will become an eigenfunction and we will have degeneracy. In the present case, to each eigenvalue $\lambda = n^2$ there correspond two eigenfunctions sin nx and cos nx.

VI. Boundary Conditions for an Infinite Interval

When p(x) becomes zero or q(x) becomes infinite at the endpoints, or when the interval is infinite, the endpoints are termed singular, and the boundary conditions must be examined more closely. The problems of interest in quantum mechanics are almost always singular in this sense. The necessity for reformulation is apparent from the fact that in the singular case, if u(x) is a solution of the differential equation (5), the limits of u(x) or of u'(x) generally do not exist at the endpoints of the interval. Consequently, the boundary conditions (7) are not applicable. In particular, it is known that sometimes the mere requirement of quadratic integrability is a sufficient boundary condition. This was elucidated by Weyl[10].

It turns out that the boundary conditions at singular endpoints are best understood by considering the eigenvalue problem for complex values of λ, as we did in the previous sections. The essential results are as follows: Suppose p(x) is continuous and greater than zero everywhere in the open interval $x_1 < x < x_2$. If $x_1 = -\infty$ or $x_2 = \infty$, or if p(x) vanishes at $x = x_1$ or at $x = x_2$, then $x = x_1$ and $x = x_2$ are singular points of the differential equation.

Let x_3 be any point in the interval (x_1,x_2) and let $w_1(x,\lambda)$ and $w_2(x,\lambda)$ be solutions of Eq. (5) satisfying the conditions $w_1(x_3) = 1$, $w_1'(x_3) = 0$ and $w_2(x_3) = 0$, $w_2'(x_3) = 1$ respectively.

Consider those solutions of Eq. (5) which satisfy the condition

$$u'(x',\lambda) + \gamma\, u(x',\lambda) = 0,$$

where x' is some fixed point between x_3 and x_2. Since the general solution of Equation (5), except for a constant factor, is

$$u(x,\lambda) = w_1(x,\lambda) + \eta\, w_2(x,\lambda) ,$$

we have

$$w_1'(x',\lambda) + \eta\, w_2'(x',\lambda) + \gamma w_1(x',\lambda) + \gamma\eta\, w_2(x',\lambda) = 0 \quad .$$

From this equation it follows that

$$\eta = \frac{\gamma w_1(x',\lambda) + w_1'(x',\lambda)}{\gamma w_2(x',\lambda) + w_2'(x',\lambda)} \quad . \tag{52}$$

If γ goes over all real values from $-\infty$ to $+\infty$, then the values of η given by Eq. (52) will, for fixed x', describe a circle in the complex η-plane.

Weyl showed that if λ is not real, the circle defined by Eq. (52) for $x' = x_4$ will contain the circle defined for $x' = x_5$ if $x_4 > x_5$. As x' approaches x_2, the circles either shrink down to a limit circle or to a limit point. In the first case it can be shown that for every real or complex value of η, we have

$$\int_{x_3}^{x_2} dx\, |u(x,\lambda)|^2 < \infty \quad . \tag{53}$$

In the second case there will exist one and only one value of η such that Eq. (53) is satisfied.

Since at an endpoint in the limit-point case there is only one quadratically integrable solution of the differential equation, we need not and in fact can not impose a boundary condition on the solution there. The mere requirement of quadratic integrability determines the solution uniquely. Note that these statements are valid only for complex values of λ; when λ is real there may be no solutions which are quadratically integrable. For example, consider the equation

$$u'' + \lambda u = 0 \tag{54}$$

in the interval $(-\infty, \infty)$. If the imaginary part of λ is positive, then $e^{i\sqrt{\lambda}x}$ is quadratically integrable at $+\infty$, while $e^{-i\sqrt{\lambda}x}$ is quadratically integrable at $-\infty$. Since no other solutions are quadratically integrable, it is clear that $\pm\infty$ are limit-point cases. When λ is real there is no quadratically integrable solution of (54).

On the other hand, in the limit-circle case there are an infinite number of solutions which are quadratically integrable. In order to specify the domain on which L acts so as to make L hermitian, it is absolutely necessary to specify an appropriate boundary condition at the endpoints. Once this is done, the well-known theorems about the spectrum of the operator can be used, and the orthogonality of the eigenfunctions follows automatically. These considerations would have greatly simplified some recent work by Case[11] on singular potentials.

We may summarize the discussion of this section as follows: In the limit-point case, the mere requirement of quadratic integrability will determine uniquely the solutions and the Green's function for complex values of λ. By analytic continuation we will get the solutions and the Green's function for real values of λ. In the limit-circle case boundary conditions must be given at both endpoints, and then we proceed as in the case of the finite interval.

VII. Expansion Theorem. Illustrations for an Infinite Interval

We now illustrate the manner in which the considerations of Section V are combined with Eq. (36) to obtain the normalized eigenfunctions when the spectrum is continuous.

A. Fourier integral.

Consider again the operator $L = -\frac{d^2}{dx^2}$, over the interval $-\infty < x < \infty$. Both endpoints are now singular. A general solution of Eq. (5) for arbitrary complex λ is

$$u(x,\lambda) = e^{i\sqrt{\lambda}x} + \gamma e^{-i\sqrt{\lambda}x} \tag{55}$$

(see Eq. (52)). Define $\sqrt{\lambda}$ so that it is real and positive on the positive real λ axis. This implies that if $\lambda = |\lambda| e^{i\theta}$, then $\lambda^{1/2} = |\lambda|^{1/2} e^{i\theta/2}$, $0 \leq \theta < 2\pi$. For non-real λ, Im $\lambda > 0$, and the only quadratically integrable solution as $x \to \infty$ is $\gamma = 0$ in (55) above. In other words, we have a limit point at $x = \infty$.

There is similarly a limit point at $x = -\infty$, the only permitted solution at that endpoint being $u(x,\lambda) = e^{-i\sqrt{\lambda}x}$. We have therefore

$$u_1(x,\lambda) = e^{-i\sqrt{\lambda}x},$$

$$u_2(x,\lambda) = e^{i\sqrt{\lambda}x}, \tag{56}$$

$$W(u_1,u_2) = 2i\sqrt{\lambda},$$

and then the Green's function is

$$x < x' : G(x,x',\lambda) = -\frac{e^{-i\sqrt{\lambda}x}\, e^{i\sqrt{\lambda}x'}}{2i\sqrt{\lambda}},$$

$$x > x' : G(x,x',\lambda) = -\frac{e^{i\sqrt{\lambda}x}\, e^{-i\sqrt{\lambda}x'}}{2i\sqrt{\lambda}}. \tag{57}$$

The Wronskian has no poles, but there is a branch-point singularity at $\lambda = 0$, and consequently $G(x,x',\lambda)$ is not a single-valued function of λ. Since we have defined λ in the range $0 \leq \arg\lambda < 2\pi$ only, we may draw a cut along the positive real λ axis and then we have, when $x < x'$,

$$-\frac{1}{2\pi i}\int_C d\lambda\, G(x,x',\lambda) = \frac{1}{2\pi i}\int_C d\lambda\, \frac{e^{i\sqrt{\lambda}(x'-x)}}{2i\sqrt{\lambda}} \tag{58}$$

with the contour as in Fig. 2. Explicitly calculating the integrals along

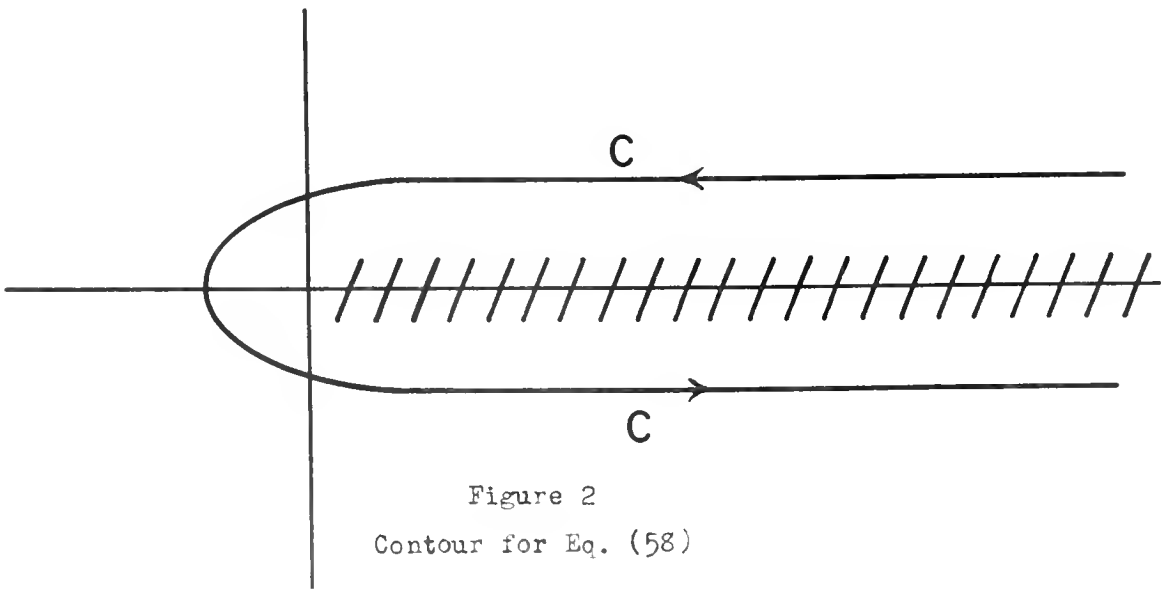

Figure 2
Contour for Eq. (58)

Cross-hatching shows cut along positive real axis.

the upper and lower sides of the cut, we obtain

$$(59)\quad -\frac{1}{2\pi i}\int_C d\lambda\, G(x,x',\lambda) = \frac{1}{4\pi}\int_0^\infty d\lambda\, \frac{e^{i\sqrt{\lambda}\,(x'-x)}}{\sqrt{\lambda}} + \frac{1}{4\pi}\int_0^\infty d\lambda\, \frac{e^{-i\sqrt{\lambda}\,(x'-x)}}{\sqrt{\lambda}} .$$

On the right side of Eq. (59), λ is real and positive. We infer that the spectrum is contimous and runs from 0 to ∞, and that there are two eigenfunctions for each value of λ, namely

$$(60)\quad u_a(x,\lambda) = \frac{1}{\sqrt{4\pi}}\,\frac{e^{i\sqrt{\lambda}\,x}}{(\lambda)^{1/4}}$$

$$u_b(x,\lambda) = \frac{1}{\sqrt{4\pi}}\,\frac{e^{-i\sqrt{\lambda}\,x}}{(\lambda)^{1/4}} .$$

The functions u_a and u_b of Eq. (60) are properly normalized. The corresponding expansion theorem is

$$(61)\quad f(x) = \frac{1}{4\pi}\int_0^\infty d\lambda\, \frac{e^{i\sqrt{\lambda}\,x}}{\sqrt{\lambda}} \int_{-\infty}^\infty dx'\, f(x')e^{-i\sqrt{\lambda}x'} + \frac{1}{4\pi}\int_0^\infty d\lambda\, \frac{e^{-i\sqrt{\lambda}\,x}}{\sqrt{\lambda}}\int_{-\infty}^\infty dx'\, f(x')e^{i\sqrt{\lambda}x'} .$$

If we introduce $k = \sqrt{\lambda}$, Eq. (61) takes the more familiar form

$$(62)\quad f(x) = \frac{1}{2\pi}\int_{-\infty}^\infty dk\, e^{ikx}\int_{-\infty}^\infty dx'\, f(x')\, e^{-ikx'} .$$

Because of the degeneracy, different sets of eigenfunctions exist which lead to alternative forms of the expansion theorem. Thus Eq. (59) could be written as

$$(63)\quad -\frac{1}{2\pi i}\int_C d\lambda\, G(x,x',\lambda) = \frac{1}{2\pi}\int_0^\infty d\lambda\, \frac{\cos\sqrt{\lambda}\,(x'-x)}{\sqrt{\lambda}}$$

$$= \frac{1}{2\pi}\int_0^\infty \frac{d\lambda}{\sqrt{\lambda}}\left[\cos x\sqrt{\lambda}\,\cos x'\sqrt{\lambda} + \sin x\sqrt{\lambda}\,\sin x'\sqrt{\lambda}\right]$$

Consequently another set of normalized eigenfunctions is

$$u_c(x,\lambda) = \frac{1}{\sqrt{2\pi}} \frac{\sin x\sqrt{\lambda}}{(\lambda)^{1/4}}$$

(64)

$$u_d(x,\lambda) = \frac{1}{\sqrt{2\pi}} \frac{\cos x\sqrt{\lambda}}{(\lambda)^{1/4}} ,$$

and the corresponding expansion theorem is

$$f(x) = \frac{1}{2\pi}\int_0^\infty d\lambda \frac{\sin x\sqrt{\lambda}}{\sqrt{\lambda}} \int_{-\infty}^{\infty} dx' f(x') \sin x'\sqrt{\lambda}$$

(65)

$$+ \frac{1}{2\pi}\int_0^\infty d\lambda \frac{\cos x\sqrt{\lambda}}{\sqrt{\lambda}} \int_{-\infty}^{\infty} dx' f(x')\cos x'\sqrt{\lambda} .$$

If we put $\lambda = k^2$, then

$$f(x) = \frac{1}{\pi}\int_0^\infty dk \int_{-\infty}^{\infty} dx' f(x') \cos k(x-x'). \tag{66}$$

Suppose the interval is $0 \leq x < \infty$. There is still a limit point at $+\infty$, but at $x = 0$ we have a limit-circle case. We impose the boundary condition $u = 0$ at $x = 0$. We have now

$$u_1(x,\lambda) = \sin \sqrt{\lambda}\, x$$

$$u_2(x,\lambda) = e^{i\sqrt{\lambda}x}$$

$$W(u_1,u_2) = -\sqrt{\lambda}$$

(67)

$$x < x' : G(x,x',\lambda) = \frac{\sin x\sqrt{\lambda}\, e^{i\sqrt{\lambda}x'}}{\sqrt{\lambda}}$$

$$x > x' : G(x,x',\lambda) = \frac{e^{i\sqrt{\lambda}x} \sin x'\sqrt{\lambda}}{\sqrt{\lambda}}$$

$$-\frac{1}{2\pi i}\int_C d\lambda\, G(x,x',\lambda) = -\frac{1}{2\pi i}\int_C \frac{d\lambda}{\sqrt{\lambda}} \sin x\sqrt{\lambda}\, e^{i\sqrt{\lambda}x'} . \tag{68}$$

The contour, the cut, and the definition of $\sqrt{\lambda}$ are as in Fig. 2 and Eq. (58). From Eq. (68) after integrating along the upper and the lower sides of the cut, we have

$$-\frac{1}{2\pi i}\int_C d\lambda G(x,x',\lambda) = -\frac{1}{2\pi i}\int_\infty^0 \frac{d\lambda}{\sqrt{\lambda}} \sin x\sqrt{\lambda}\, e^{ix'\sqrt{\lambda}} - \frac{1}{2\pi i}\int_0^\infty \frac{d\lambda}{\sqrt{\lambda}} \sin x\sqrt{\lambda}\, e^{-ix'\sqrt{\lambda}}$$

$$= \frac{1}{\pi}\int_0^\infty \frac{d\lambda}{\sqrt{\lambda}} \sin x\sqrt{\lambda} \sin x'\sqrt{\lambda}\ . \tag{69}$$

In the last equality of (69), λ is real and positive. Eq. (69) shows that the spectrum extends from 0 to ∞, and that there is only one eigenfunction for each λ, namely

$$u(x,\lambda) = \frac{1}{\sqrt{\pi}} \frac{\sin x\sqrt{\lambda}}{(\lambda)^{1/4}}\ . \tag{70}$$

Using the expansion theorem, we find that in the interval $0 \le x < \infty$

$$f(x) = \frac{1}{\pi}\int_0^\infty d\lambda \frac{\sin x\sqrt{\lambda}}{\sqrt{\lambda}} \int_0^\infty dx'\, f(x') \sin x'\sqrt{\lambda} \tag{71}$$

or, if we put $\lambda = k^2$,

$$f(x) = \frac{2}{\pi}\int_0^\infty dk \sin kx \int_0^\infty dx'\, f(x') \sin kx'\ . \tag{72}$$

B. Alternative representations of outgoing Green's function.

In order to bring out some important points we shall obtain some alternative representations for the Green's function. Consider the following integral over a circle of radius R:

$$G_R = \frac{1}{2\pi i} \oint d\lambda' \frac{G(x,x',\lambda')}{\lambda' - \lambda}\ , \tag{73}$$

where $G(x,x',\lambda')$ is the Green's function. We assume that as R approaches infinity, G_R approaches zero; then evaluating G_R by residues, we have

$$G(x,x',\lambda) = -\frac{1}{2\pi i}\int_C \frac{d\lambda' G(x,x',\lambda')}{\lambda' - \lambda}\ , \tag{74}$$

where C is a contour which encloses all the singularities, poles, or branch cuts of the Green's function but does not enclose the point λ. As an illustration,

consider the Green's function given by (57). We have

$$(75) \qquad G(x,x',\lambda) = -\frac{1}{4\pi}\int_C d\lambda' \, \frac{e^{i\sqrt{\lambda'}\,|x'-x|}}{(\lambda'-\lambda)\sqrt{\lambda'}} ,$$

where C is a contour enclosing the branch cut. In order that G_R approach zero as R approaches infinity, the cut must be chosen so that the imaginary part of $\sqrt{\lambda'}$ is positive. This implies that the cut must be taken along the positive real axis and that $0 < \arg \lambda' < 2\pi$. In other words, the contour C in the complex λ'-plane is precisely the contour of Fig. 2. Put $\lambda' = k^2$ in (75) and it becomes

$$(76) \quad G(x,x',\lambda) = \frac{1}{2\pi}\int_0^\infty dk \left[\frac{e^{ik|x'-x|}}{k^2-\lambda} + \frac{e^{-ik|x'-x|}}{k^2-\lambda}\right] = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk \, \frac{\cos k\,(x'-x)}{(k-\sqrt{\lambda})(k+\sqrt{\lambda})} .$$

Equation (76) is valid for all λ such that $0 < \arg \lambda < 2\pi$. Consequently, the pole at $k = \sqrt{\lambda}$ is in the upper half of the complex k-plane while the pole at $k = -\sqrt{\lambda}$ is in the lower half of that plane. Note that k runs along the real axis by virtue of the fact that we put $\lambda' = k^2$ in (75), where λ' ran along the real positive axis on either side of the cut. However, the contour in the k-plane may be deformed provided no singularities are crossed. By deforming the contour downward to the right of the origin, and upward to the left of the origin, it is seen that the last integral in Eq. (76) defines an analytic function of λ as the imaginary part of λ approaches zero for positive λ. Consequently, for real $\lambda > 0$, the contour in the k-plane must be the one shown in Fig. 3, this being the only one for which Eq. (76) is valid when $G(x,x',\lambda)$ is the Green's function of Eq. (57). This Green's function would ordinarily be termed the outgoing Green's function, so we have obtained an integral representation, with correctly chosen contour, of the outgoing Green's function for the operator $L = -\frac{d^2}{dx^2}$.

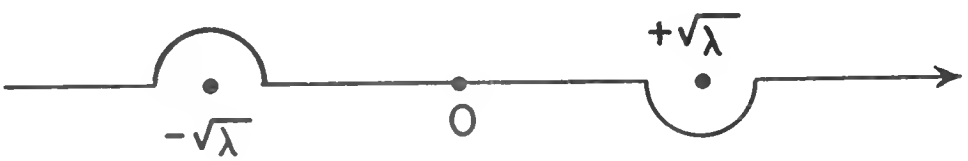

Fig. 3

There is another interesting point about the representation of $G(x,x',\lambda)$ given in (76). The last integral contains $\cos k(x-x')$ and this seems to indicate that $G(x,x',\lambda)$ is made up of outgoing waves $e^{ik(x-x')}$ and also incoming waves $e^{-ik(x-x')}$. However, we can easily see that the incoming part is zero when we evaluate

$$\frac{1}{4\pi}\int_{-\infty}^{\infty}\frac{e^{-ik(x-x')}}{k^2-\lambda}\,dk.$$

For x approaching ∞, the contour may be closed in the lower half-plane, and then the integral becomes

$$\frac{e^{i\sqrt{\lambda}\,(x-x')}}{4i\sqrt{\lambda}},$$

an outgoing term. This result demonstrates that by merely glancing at an integral it is not possible to determine its asymptotic behavior, or whether it is made up of outgoing or incoming waves. This statement is obvious, but its implications have not always been understood, especially in many-particle problems where different representations of the Green's function are possible.

VIII. Transmission and Reflection Coefficients in One Dimension

We return now to the discussion of scattering in one dimension. We are interested in a solution of the equation

$$-\frac{d^2\psi}{dx^2}+q\psi=\lambda\psi \tag{77}$$

for real λ. The solution $\psi(x)$ should be of the form

$$\psi(x)=e^{i\sqrt{\lambda}\,x}+\phi(x), \tag{78}$$

where $\phi(x)$ is everywhere outgoing at infinity, that is,

$$\begin{aligned}\phi(x)&\sim A\,e^{i\sqrt{\lambda}\,x}\quad,\ x\to\infty\\ \phi(x)&\sim B\,e^{-i\sqrt{\lambda}\,x}\quad,\ x\to-\infty.\end{aligned} \tag{79}$$

The physical interpretation of the problem is this: a plane wave $e^{i\sqrt{\lambda}\,x}$ comes in from $-\infty$, is scattered by the potential $q(x)$, and thereby causes the appearance of an outgoing wave $A\,e^{i\sqrt{\lambda}\,x}$ at $+\infty$, and an outgoing wave $B\,e^{-i\sqrt{\lambda}\,x}$ at $-\infty$. It should be realized that the assumptions (78) and (79) about the behavior of $\psi(x)$ are valid only if $q(x)$ is not too large at infinity. For example, if $q(x)$ were the Coulomb potential $1/x$, then (78) and (79) would be impossible.

Sufficient conditions for the validity of (78) and (79) are that $q(x)$ vanish outside some finite interval or, more generally, that

$$\int_{-\infty}^{\infty} |q(x)|\, dx < \infty. \tag{80}$$

We assume (80) and consider what happens when a plane wave $e^{i\sqrt{\lambda}\, x}$ comes in from minus infinity. Some of it will be transmitted to plus infinity, while the rest of it will be reflected back to minus infinity. Let $u_2(x)$ represent the solution of (77) which has these properties. Since we are interested only in the stationary case, we may write the asymptotic relations

$$\begin{aligned} u_2(x) &\sim e^{i\sqrt{\lambda}x} + R_- e^{-i\sqrt{\lambda}x}, \quad x \to -\infty \\ u_2(x) &\sim T_- e^{i\sqrt{\lambda}\, x}, \quad x \to \infty, \end{aligned} \tag{81}$$

where R_- is the reflection amplitude coefficient and T_- is the transmission amplitude coefficient. Because (77) is a real equation, the conjugate to $u_2(x)$, namely $u_2^*(x)$, is also a solution of (77), and from (81) we have

$$\begin{aligned} u_2^*(x) &\sim e^{-i\sqrt{\lambda}\, x} + R_-^* e^{i\sqrt{\lambda}\, x}, \quad x \to -\infty \\ u_2^*(x) &\sim T_-^* e^{-i\sqrt{\lambda}\, x}, \quad d \to \infty. \end{aligned} \tag{82}$$

We have mentioned before that the Wronskian of any two solutions of (77) is constant for all values of x. Let us apply this result to the solutions $u_2(x)$ and $u_2^*(x)$. We have

$$W\left[u_2^*(x), u_2(x)\right]_{-\infty} = u_2^*(x)u_2'(x) - u_2^{*\prime}(x)u_2(x)\Big|_{-\infty} = +2i\sqrt{\lambda}\,(1-|R_-|^2)$$

$$W\left[u_2^*(x), u_2(x)\right]_{+\infty} = +2i\sqrt{\lambda}\,|T_-|^2,$$

and therefore

$$1 - |R_-|^2 = |T_-|^2, \text{ or } |R_-|^2 + |T_-|^2 = 1. \tag{83}$$

Thus the sum of the reflection and transmission is equal to unity. Note that the quantum-mechanical current is defined as $\frac{\hbar}{2mi} W(u_2^*, u_2)$, and that because of the properties of the Wronskian this current is independent of x.

Similar results hold in the case of waves coming in from $+\infty$. We may assume

$$(84)\qquad \begin{aligned} u_1(x) &\sim e^{-i\sqrt{\lambda}\,x} + R_+ e^{i\sqrt{\lambda}\,x}, \quad x \longrightarrow \infty \\ u_1^*(x) &\sim T_+ e^{-i\sqrt{\lambda}\,x}, \quad x \longrightarrow -\infty , \end{aligned}$$

where R_+ is the reflection amplitude coefficient and T_+ is the transmission amplitude coefficient for waves coming in from $+\infty$. As before, since (77) is real, $u_1^*(x)$ is a solution, and the Wronskian of u_1^*, u_1 is constant for all values of x. We have

$$\begin{aligned} u_1^*(x) &\sim e^{i\sqrt{\lambda}\,x} + R_+^* e^{-i\sqrt{\lambda}\,x}, \quad x \to \infty \\ u_2^*(x) &\sim T_+^* e^{i\sqrt{\lambda}\,x}, \quad x \to \infty \end{aligned}$$

$$W\left[u_1^*, u_1\right]_{\infty} = -2i\sqrt{\lambda}\,\left[1 - |R_+|^2\right]$$

$$W\left[u_1^*, u_1\right]_{-\infty} = -2i\sqrt{\lambda}\,|T_+|^2 ,$$

and therefore

$$(85)\qquad 1 - |R_+|^2 = |T_+|^2 \text{ or } |R_+|^2 + |T_+|^2 = 1 .$$

Another important relation may be obtained by considering the Wronskian of u_1 and u_2. Since u_1 and u_2 are both so solutions of (77) we have

$$W\left[u_1, u_2\right]_{\infty} = W\left[u_1, u_2\right]_{-\infty} .$$

Then

$$W\left[u_1, u_2\right]_{\infty} = +2i\sqrt{\lambda}\,T_- ,$$

$$W\left[u_1, u_2\right]_{-\infty} = +2i\sqrt{\lambda}\,T_+ ;$$

therefore we get

$$(86)\qquad T_- = T_+ .$$

which states the reciprocity relation that the transmission coefficient for waves coming from the left is equal to the transmission coefficient for waves coming from the right.

Our final relation is obtained by considering $W[u_1^*, u_2]$. We have

$$W[u_1^*, u_2]_{\infty} = 2i\sqrt{\lambda}\, R_+^* T_-$$

$$W[u_1^*, u_2]_{-\infty} = -2i\sqrt{\lambda}\, R_- T_+^* ,$$

and therefore

$$R_+^* T_- + R_- T_+^* = 0 . \tag{87}$$

It is worthwhile noticing that the functions u_1 and u_2 are unique. Suppose there were two functions u_1 and $\bar{u}_1$ which had the same properties; then $u_1 - \bar{u}_1$ would be a solution of (77) which is outgoing at both $+\infty$ and $-\infty$. For one-dimensional problems the impossibility of such non-vanishing solutions for real positive values of λ can be easily established[12]. Notice also that u_2/T_- and u_1/T_+ are analytic functions of λ.

A. The scattering matrix.

We now consider waves coming in from both $-\infty$ and $+\infty$. Suppose that $\psi(x)$ contains a wave $a_- e^{i\sqrt{\lambda}x}$ coming in from $-\infty$ and a wave $a_+ e^{-i\sqrt{\lambda}x}$ coming in from $+\infty$. Since any linear combination of u_1 and u_2 is also a solution of (77), we have

$$\psi(x) = a_- u_2(x) + a_+ u_1(x),$$

and then from (81) and (85) we find that the scattered outgoing waves are

$$\begin{aligned} b_+ e^{-i\sqrt{\lambda}x} &= (a_- R_- + a_+ T_+)\, e^{-i\sqrt{\lambda}x} , \quad x \to -\infty \\ b_- e^{+i\sqrt{\lambda}x} &= (a_- T_- + a_+ R_+)\, e^{i\sqrt{\lambda}x} , \quad x \to +\infty . \end{aligned} \tag{88}$$

The current is, as stated previously, $\frac{\hbar}{2mi} W(\psi^*, \psi)$. However it is convenient and physically natural to think of the current as consisting of incoming and outgoing parts, the incoming current at $x = +\infty$ for example being defined by using in the Wronskian not the complete solution ψ but only that portion which is incoming

at $x = +\infty$. The currents may be interpreted in this way because there is no interference between the incoming and outgoing portions of the current. To illustrate, at $x = +\infty$ the outgoing current u_o is proportional to $e^{i\sqrt{\lambda}\,x}$, the incoming current u_i is proportional to $e^{-i\sqrt{\lambda}x}$, and the interference terms in the current are proportional to $W(u_i^*, u_o) = W(e^{i\sqrt{\lambda}x}, e^{i\sqrt{\lambda}x})$ and to $W(u_o^*, u_i) = (e^{-i\sqrt{\lambda}x}, e^{-i\sqrt{\lambda}x})$, which vanish. Consequently the currents at $x = +\infty$ and $x = -\infty$ are

$$\frac{\hbar}{2mi} W(\psi^*, \psi)_{+\infty} = \frac{\hbar}{2mi} W\left(a_+^* e^{i\sqrt{\lambda}x} + b_-^* e^{-i\sqrt{\lambda}x},\ a_+ e^{-i\sqrt{\lambda}x} + b_- e^{i\sqrt{\lambda}x}\right)_{+\infty}$$

$$= \frac{\hbar}{m}\sqrt{\lambda}\ \left(-|a_+|^2 + |b_-|^2\right),$$

$$\frac{\hbar}{2mi} W(\psi^*, \psi)_{-\infty} = \frac{\hbar}{2mi} W\left(a_-^* e^{-i\sqrt{\lambda}x} + b_+^* e^{i\sqrt{\lambda}x},\ a_- e^{i\sqrt{\lambda}x} + b_+ e^{-i\sqrt{\lambda}x}\right)_{-\infty}$$

$$= \frac{h}{m}/\lambda\ \left(|a_-|^2 - |b_+|^2\right).$$

It is seen that the current at $x = +\infty$ or $x = -\infty$ is the difference between the incoming and outgoing parts, in the sense explained above. Moreover, equating the Wronskians at $+\infty$ and $-\infty$,

$$\frac{\hbar}{m}\sqrt{\lambda}\ \left(|a_-|^2 + |a_+|^2\right) = \frac{\hbar}{m}\sqrt{\lambda}\ \left(|b_+|^2 + |b_-|^2\right).$$

Thus we have proved that the total outgoing current equals the total incoming current, a result which is essential for a consistent interpretation in terms of incoming and outgoing currents.

We may express (88) very simply in matrix notation. We have

$$\begin{pmatrix} b_+ \\ b_- \end{pmatrix} = S \begin{pmatrix} a_+ \\ a_- \end{pmatrix},$$

where S is the matrix

(89)
$$\begin{pmatrix} T_+ & R_- \\ R_+ & T_- \end{pmatrix}.$$

S is called the collision or scattering matrix and is defined so as to equal the unit matrix when q is zero in (77). From (83), (85), and (87) we obtain the relation

$$S\,S^{\dagger} = I,$$

where $S^{\dagger}$ is the complex conjugate of the transpose of S, and I is the unit matrix. This relation shows that S is unitary. This property of S could also have been deduced from the fact that

$$|b_+|^2 + |b_-|^2 = |a_+|^2 + |a_-|^2 .$$

Note that from (86) and (87) it follows that

$$|T_+|^2 = |T_-|^2 \text{ and } |R_+|^2 = |R_-|^2 ,$$

which shows that the reflection and transmission coefficients do not depend on whether the wave comes from the left or right.

Up to this point we have assumed that λ is real in equation (77) and the subsequent analysis. If λ is complex, u_1^* and u_2^* are no longer solutions of the equation (77) for the same eigenvalue λ as are u_1 and u_2; consequently the relations (83),(85), and (87) are no longer valid. Only the relation (86) remains.

We may, however, continue to define the matrix S of (89) formally as the analytic continuation into the complex λ-plane of the scattering matrix obtained for real values of λ. Because the relations (83), (85), and (87) are not valid, S will no longer be unitary for complex values of λ. It can easily be shown that T_+, T_-, R_+, and R_- are analytic functions of λ in the upper and lower half-planes. Thus the only possible singularities of the scattering matrix are on the real axis.

We shall show that the singularities of the scattering matrix contain the singularities of the Green's function $G(x,x',\lambda)$ for the operator L and therefore also for the eigenvalues of L. The solution of (77) which for complex λ is quadratically integrable at $x = +\infty$ is proportional to $u_2(x,\lambda)$, i.e. to the solution which in this section has been called outgoing at $+\infty$. In fact the function u_2/T_- behaves like $e^{i\sqrt{\lambda}\,x}$ at $+\infty$. Similarly the function u_1/T_+ behaves like $e^{-i\sqrt{\lambda}\,x}$ at $-\infty$. Thus, since

$$W\left[u_1/T_+,\ u_2/T_-\right] = \frac{1}{T_+T_-}\ W[u_1,u_2]_{-\infty} = \frac{2i\sqrt{\lambda}}{T_-} ,$$

we have as in section VII

$$G(x,x',\lambda) = - \frac{e^{-i\sqrt{\lambda}\,x}\; e^{i\sqrt{\lambda}\,x'}}{W\left[u_1/T_+, u_2/T_-\right]} = - \frac{e^{i\sqrt{\lambda}\,(x'-x)}}{2i\sqrt{\lambda}}\; T_-(\lambda)\,,$$

for $x < x'$, x approaching $-\infty$ and x' approaching $+\infty$.

We shall now derive integral expressions for the elements of the scattering matrix. Consider the function u_2. We know that

$$u_2 = e^{i\sqrt{\lambda}\,x} + \phi_2(x)\,,$$

where $\phi_2(x)$ is outgoing at both $+\infty$ and $-\infty$. This expression is substituted for u_2 in (77) and we get

$$- \frac{d^2\phi_2}{dx^2} - \lambda\phi_2 = -qu_2\,.$$

Now we use the outgoing wave Green's function Eq. (57) for the left side and obtain

$$\phi_2 = \frac{1}{2i\sqrt{\lambda}} \int e^{i\sqrt{\lambda}\,|x-x'|}\; q(x')\; u_2(x')\,dx'$$

or

$$u_2 = e^{i\sqrt{\lambda}\,x} + \frac{1}{2i\sqrt{\lambda}} \int_{-\infty}^{\infty} e^{i\sqrt{\lambda}\,|x-x'|}\; q(x')u_2(x')dx'\,.$$

Now let x approach first $-\infty$ and then $+\infty$. We find that

$$e^{i\sqrt{\lambda}\,x} + R_-\, e^{-i\sqrt{\lambda}\,x} = e^{i\sqrt{\lambda}\,x} + \frac{e^{-i\sqrt{\lambda}\,x}}{2i\sqrt{\lambda}} \int_{-\infty}^{\infty} e^{i\sqrt{\lambda}\,x'} qu_2 dx'$$

and

$$T_-\, e^{i\sqrt{\lambda}\,x} = e^{i\sqrt{\lambda}\,x} + \frac{e^{i\sqrt{\lambda}\,x}}{2i\sqrt{\lambda}} \int_{-\infty}^{\infty} e^{-i\sqrt{\lambda}\,x'}\; qu_2\; dx';$$

consequently

$$T_- = 1 + \frac{1}{2i\sqrt{\lambda}} \int_{-\infty}^{\infty} e^{-i\sqrt{\lambda}\,x}\; qu_2\; dx$$

(90)

$$R_- = \frac{1}{2i\sqrt{\lambda}} \int_{-\infty}^{\infty} e^{i\sqrt{\lambda}\,x}\; qu_2\; dx\,.$$

Similarly we obtain

$$T_+ = 1 + \frac{1}{2i\sqrt{\lambda}} \int_{-\infty}^{\infty} e^{i\sqrt{\lambda}\, x}\, q u_1\, dx$$

(91)

$$R_+ = \frac{1}{2i\sqrt{\lambda}} \int_{-\infty}^{\infty} e^{-i\sqrt{\lambda}\, x}\, q u_1\, dx \quad .$$

Reference 13 gives a much expanded treatment of the scattering problem. In this work, it is shown that it is also possible to derive results such as (90) and (91) by means of formal symbolic operator techniques[13,14] . We have preferred, however, to demonstrate (90) and (91) directly from the differential equation in order to avoid any difficulties about the meaning of the operators that must otherwise be symbolically defined[13,14] . We intend, in our next report, to consider the scattering matrix for a three-dimensional particle, in which case the corresponding one-dimensional (radial) equation covers the semi-infinite interval $0 \leq r < \infty$ instead of the fully infinite interval which we have been considering. There exist numerous papers on the subject of the scattering matrix in the three-dimensional case; those by Ma[15] and van Kampen[16] contain results and references which are of interest.

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